Binding Energies of Open-Shell Nuclei

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The binding energies of open-shell nuclei ($2s$-$1d$) are calculated from the approximate Hartree-Fock solution along with the use of the projection technique, both for the Yale potential and for a nonlocal separable potential. It is observed that though the Yale potential gives better binding than the nonlocal potential does, it still gives lower values than the experimental numbers, as was the case for the O^{16} nucleus.

I. INTRODUCTION

IT is well known that because of the very strong repulsive nature of the short-range internucleon forces, the simple perturbation methods and the variational methods are not directly applicable. However, various different approaches have been suggested in the literature to cope with this difficulty.[1] Following Villars[2] approach, Shakin and Waghmare[3] obtained the effective Hamiltonian by making a unitary transformation on the unperturbed wave functions. Using a rather different approach, Kuo and Brown[4] have also utilized an effective interaction of a pair of nucleons inside a nucleus. These approaches thus provide a way to carry out Hartree-Fock (HF) calculations for nuclei even though the nucleon-nucleon interaction is singular.

In this paper we will use the Yale potential,[5] since its effective-interaction matrix elements are available.[6] Because of a difficulty in the construction of good antisymmetric angular momentum states for open-shell nuclei, the authors of Refs. 4 and 6 restrict their calculations to doubly-closed-shell nuclei. The second difficulty that one encounters with open-shell nuclei is that of renormalization of the effective interaction for the outer nucleons due to core polarization. This latter difficulty has been investigated in Ref. 4 in the case of the O^{18} nucleus. Our aim here is to determine the binding energies of $2s$–$1d$-shell nuclei using the Yale potential. We avoid the first difficulty by using the projection technique,[7] and the second by using a perturbation method based on the HF solution for the O^{16} nucleus.

A necessary theoretical formulation is carried out in Sec. II. Results of the calculations are presented in Sec. III. Section IV summarizes the results.

II. THEORETICAL FORMULATION

The Hamiltonian of a system of nucleons interacting via a free nucleon-nucleon interaction can be transformed by a unitary transformation into an effective Hamiltonian $\bar{H}$.[2] Its approximate form as given in Ref. 5 is

$$\bar{H}\approx\sum_{mn}(n|p^2/2m|m)a_n^\dagger a_m + \tfrac{1}{2}\sum_{mnlp}(mn|v_{\text{eff}}|lp)a_m^\dagger a_n^\dagger a_p a_l, \quad (1)$$

where the necessary matrix elements of v_{eff} are also given. Since we make use of the projection technique to calculate the binding energies of the open-shell nuclei, we should have to carry out deformed HF calculations based on the Hamiltonian in Eq. (1). Any such calculations certainly would be very involved. In the following, we use an approximate scheme to reduce the calculations to manageable size.

A. Approximate Hartree-Fock Solution

One expects the single-particle orbitals of the total HF solution of open-shell nuclei to be deformed. However, the core orbitals should have essentially spherical symmetry. Let us consider a nucleus of A core particles and N outer nucleons. We now look for an approximation to the total HF problem that will reduce it to two separate HF calculations. One is the HF solution for the core nucleons, the results of which are available.[5] Another is the deformed HF calculation for outer nucleons. In the following, we investigate the single-particle energies and the two-body interaction that should be used in the latter HF calculations. We then find the binding energies of $2s$–$1d$-shell nuclei from this approximate solution, using the projection technique.

The total HF energy from Eq. (1) is

$$E_{\text{HF}}(\psi)=E_{\text{HF}}(A)+E_{\text{HF}}(N)+\sum_{j=A+1}^{A+N}\langle\psi_j|V|\psi_j\rangle, \quad (2)$$

where $\psi_i(i=1,\cdots,A+N)$ are the orthonormal set of single-particle orbitals to be found from the minimization of Eq. (2). The other symbols in Eq. (2) are as

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[2] F. Villars, in *Proceedings of the International School of Physics, "Enrico Fermi" Course 23, 1961* (Academic Press Inc., New York, 1963).

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[4] T. S. Kuo and G. E. Brown, Nucl. Phys. **85**, 40 (1966).

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[6] C. M. Shakin, Y. R. Waghmare, and M. H. Hull, Phys. Rev. **161**, 1015 (1967).

[7] C. S. Warke and M. R. Gunye, Phys. Rev. **155**, 1084 (1967).

follows:

$$E_{\mathrm{HF}}(A)=\sum_{i=1}^{A}\langle\psi_i|\,p^2/2m|\psi_i\rangle + \tfrac{1}{2}\sum_{ij=1}^{A}\langle\psi_i\psi_j|\mathcal{V}_{\mathrm{eff}}(1-P_{ij})|\psi_i\psi_j\rangle$$

and a similar expression for $E_{\mathrm{HF}}(N)$, and

$$\langle\psi_i|\,V|\psi_i\rangle=\sum_{j=1}^{A}\langle\psi_i\psi_j|\mathcal{V}_{\mathrm{eff}}(1-P_{ij})|\psi_i\psi_j\rangle,$$

P_{ij} being the particle exchange operator.

Considering the fact that the core orbitals will remain mostly spherical if the last term is a small perturbation, the zeroth-order approximation for the core orbitals $\psi_i^{(0)}$ $(i=1,\cdots,A)$ can be obtained from the spherical HF solution of $E_{\mathrm{HF}}(A)$. From this known solution one then calculates the excited orbitals and their energies. Let us denote this HF Hamiltonian by h_0, with eigenfunctions and eigenvalues $\psi_i^{(0)}$ and ϵ_i, respectively. If one minimizes E_{HF} for the variations of $\psi_i^{(0)}(i=1,\ A)$, taking into account the last term in Eq. (2), one obtains the following equation for ψ_i:

$$(h_0+V)\psi_i=E_i\psi_i \quad (i=1,\cdots,A). \tag{3}$$

Using first-order perturbation theory, one obtains from Eq. (3)

$$\psi_i^{(1)}=\psi_i^{(0)}+(\epsilon_i-h_0)^{-1}V\psi_i^{(0)}\equiv\psi_i^{(0)}+\delta\psi_i \quad \text{for} \quad i=1,\cdots,A. \tag{4}$$

Since the HF orbitals form an orthonormal set, $\delta\psi_i$ in Eq. (4) is orthogonal to $\psi_i^{(0)}$ $(i=1,\cdots,A)$ as well as to ψ_i $(i=A+1,\cdots,A+N)$. In our problem we treat it in a certain approximate manner. As our $\psi_i^{(0)}$ are the HF solutions of $E_{\mathrm{HF}}(A)$, the change in it due to the change of $\psi_i=\psi_i^{(0)}+\delta\psi_i$ $(i=1,\cdots,A)$ is at least of second order in $\delta\psi_i$. Keeping up to linear terms in $\delta\psi_i$, we obtain from Eq. (3)

$$E_{\mathrm{HF}}(\psi)\approx E_{\mathrm{HF}}(A,\psi_i^{(0)})+E_{\mathrm{HF}}(N)+\sum_{j=1}^{A}\langle\psi_j^{(0)}|\,V|\psi_j^{(0)}\rangle + 2\sum_{j=1}^{A}\langle\delta\psi_j|\,V|\psi_j^{(0)}\rangle. \tag{5}$$

The condition that $\delta\psi_i$ be orthogonal to $\psi_i^{(0)}(i=1,\cdots,A)$ can easily be accounted for by simply excluding these orbitals in the expansion of $\delta\psi_i$ in Eq. (4). However, it is difficult to enforce the condition that $\delta\psi_i$ should be orthogonal to $\psi_i(i=A+1,\cdots,A+N)$, simply because we have not yet obtained these orbitals. At this stage we introduce an approximation that maintains this orthogonality on the average. Let $\rho_{\alpha\beta}$ be the one-particle density matrix for the outer nucleons. Then $\Sigma_\beta\rho_{\alpha\beta}^2$ is the probability that the αth state is occupied by these outer N nucleons. We define the amplitude A_α for the αth orbital to be empty as

$$A_\alpha=[1-\sum_\beta\rho_{\alpha\beta}^2]^{1/2}. \tag{6}$$

From Eqs. (4) and (6) we have

$$\delta\psi_j=\sum_{i>A}\frac{A_i}{(\epsilon_j-\epsilon_i)}\langle i|\,V|\,j\rangle\psi_i^{(0)}. \tag{7}$$

Substituting Eq. (7) into Eq. (5) and rearranging terms we obtain

$$E_{\mathrm{HF}}(\psi_i)=E_{\mathrm{HF}}(A,\psi_i^{(0)})+E_{\mathrm{HF}}{}^r(N), \tag{8}$$

where the renormalized HF energy $E_{\mathrm{HF}}{}^r(N)$ of the outer N nucleons is

$$E_{\mathrm{HF}}{}^r(N)=\sum_{j=A+1}^{A+N}\langle\psi_j|\,t|\psi_j\rangle + \tfrac{1}{2}\sum_{ij=A+1}^{A+N}\langle\psi_i\psi_j|\mathcal{V}|\psi_i\psi_j-\psi_j\psi_i\rangle. \tag{9}$$

The modified one-body potential t and the renormalized two-body interaction $\mathcal{V}$ have the following form:

$$t(i)=p_i^2/2m+\sum_{\alpha=1}^{A}(\alpha|\mathcal{V}_{\mathrm{eff}}(i,1)(1-P_{i1})|\alpha)$$

and

$$\mathcal{V}(i,j)=\mathcal{V}_{\mathrm{eff}}(i,j)+2\sum_{\alpha=1}^{A}\sum_{m>A}\frac{A_m}{(\epsilon_\alpha-\epsilon_m)} \times(m|\mathcal{V}_{\mathrm{eff}}(i,1)(1-P_{i1})|\alpha)(\alpha|\mathcal{V}_{\mathrm{eff}}(j,1) \times(1-P_{1j})|m). \tag{10}$$

The bracketed matrix element in Eq. (10) denotes

$$(m|\mathcal{V}_{\mathrm{eff}}(i,1)(1-P_{i1})|\alpha)=\int\psi_m^{*(0)}(1)\mathcal{V}_{\mathrm{eff}}(i,1) \times(1-P_{i1})\psi_\alpha^{(0)}(1)dP_1.$$

We can now obtain the deformed HF orbitals for the outer N nucleons by minimizing $E_{\mathrm{HF}}(N)$ in Eq. (9). To start with we may substitute some values for A_j

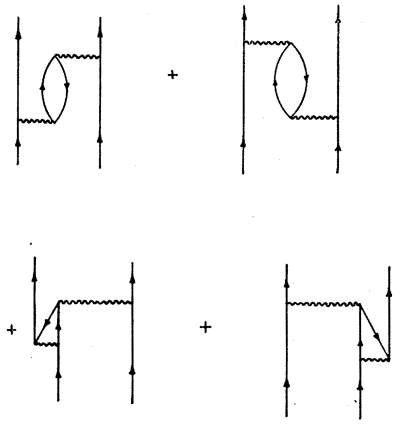

FIG. 1. Diagrams contributing to last term in Eq. (10).

and then obtain the deformed HF solution for outer nucleons. From this solution we can reconstruct A_j and iterate the process until we get a self-consistent solution. The last term in Eq. (10) is essentially the contribution of the diagrams shown in Fig. 1. The renormalized interaction in Eq. (10) is similar to Kuo and Brown's[4] core-polarization correction to obtain a model interaction.

In our formulation the core wave function has a form similar to that of a spherical doubly-closed-shell nucleus. In this case the geometrical sums involved in Eq. (10) can be carried out if one assumes that A_m does not depend on the projection of the angular momentum. After performing some straightforward angular momentum algebra, one obtains the following expression for the matrix element of $v(i,j)$:

$$\langle n_1l_1j_1n_2l_2j_2;JT|\mathcal{U}^a|n_1'l_1'j_1'n_2'l_2'j_2';JT\rangle=\langle n_1l_1j_1n_2l_2j_2,JT|\mathcal{U}_{\rm eff}{}^a|n_1'l_1'j_1'n_2'l_2'j_2'\rangle$$

$$+2\sum_{\substack{\alpha<A,m>A\\J_1T_1J_2T_2}}(\text{Phase})(2T_1+1)(2T_2+1)(2J_1+1)(2J_2+1)\begin{Bmatrix}j_1 & j_m & J_1\\ j_2 & J_2 & j_\alpha\\ J & j_2' & j_1'\end{Bmatrix}\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & T_1\\ \frac{1}{2} & T_2 & \frac{1}{2}\\ T & \frac{1}{2} & \frac{1}{2}\end{Bmatrix}A(n_m,l_m)$$

$$\times\langle n_1l_1j_1n_ml_mj_m;J_2T_2|\mathcal{U}_{\rm eff}{}^a|n_1'l_1'j_1'n_\alpha l_\alpha j_\alpha;J_2T_2\rangle\langle n_2l_2j_2n_\alpha l_\alpha j_\alpha;J_2T_2|\mathcal{U}_{\rm eff}{}^a|n_2'l_2'j_2'n_ml_mj_m;J_2T_2\rangle$$

$$\times(\epsilon_m-\epsilon_\alpha)^{-1}. \quad (11)$$

The superscript a on $\mathcal{U}$ and $\mathcal{U}_{\rm eff}$ in Eq. (11) denotes the antisymmetrized matrix elements, and

$$(\text{Phase})=(-1)^{j_2+j_2'+1+J+J_1+J_2+T+T_1+T_2}.$$

We will not quote the usual complicated expressions[5] for the matrix elements occurring in Eq. (11).

B. Correction to the Truncated HF Solution

In doing the HF calculations, one usually confines oneself to a set of harmonic-oscillator orbitals, and thereby neglects the higher configurations. In this subsection we study the effect of this approximation on the HF solution. We follow the projection-operator technique of Feshbach.[8] One knows that a minimization of the total energy of a system of nucleons with respect to a determinantal wave function, formed from the one-particle wave functions ψ_i, leads to the HF equation $h\psi=\epsilon\psi$. The wave functions ψ_i are the eigenfunctions of h with eigenvalues ϵ_i. The one-body HF Hamiltonian h is given by

$$h(i)=t(i)+\sum_\alpha(\psi_\alpha|\mathcal{U}(i,\alpha)(1-P_{i\alpha})|\psi_\alpha)$$
$$=t(i)+\sum_\alpha(\psi_\alpha|\mathcal{U}^a|\psi_\alpha), \quad (12)$$

where t and $\mathcal{U}$ are the one-body and the two-body potential. Let P be the operator that projects out the set of orbitals used in a truncated HF solution. Let us also define an orthogonal operator $Q=1-P$, so that $PQ=0$. Since P and Q project out a certain set of functions, we have $P^2=P$, and $Q^2=Q$. Writing $\psi=P\psi+Q\psi$, it is not difficult to observe from the HF equation that

$$|Q\psi\rangle=1|(\epsilon-h_{QQ})h_{QP}|P\psi\rangle$$

and

$$h_{PP}|P\psi\rangle+h_{PQ}|(\epsilon-h_{QQ})h_{QP}|P\psi\rangle=\epsilon|P\psi\rangle, \quad (13)$$

where we have used the notation $h_{PQ}=PhQ$, etc. Similarly, V in Eq. (12) can also be rewritten as

$$V=V(P,P)+V(P,Q)+V(Q,P)+V(Q,Q)\cdots, \quad (14)$$

where

$$V(P,Q)=\sum_\alpha(P\psi_\alpha|\mathcal{U}^a|Q\psi_\alpha), \quad \text{etc.}$$

From Eqs. (13) and (14) one finally obtains

$$\{h_0+V_{PP}(Q,P)+V_{PP}(Q,P)+V_{PP}(Q,Q)+h_{PQ}|(\epsilon-h_{QQ})h_{QP}\}|P\psi\rangle$$
$$=\{h_0+V'(\epsilon)\}|P\psi\rangle=\epsilon|P\psi\rangle. \quad (15)$$

In the truncated HF problem one solves the eigenvalue problem

$$h_0|P\psi_i\rangle=[t+V_{PP}(P,P)]|P\psi_i\rangle=\eta_i|P\psi_i\rangle. \quad (16)$$

From Eqs. (15) and (16) one can determine corrections to the truncated HF solution using standard perturbation theory. In this paper we have not carried out any corrections to our HF solution.

III. RESULTS

We use two sets of potentials in applying the formulation developed in Sec. II. One is the Yale potential[5] and the other a separable nonlocal s-state potential used in Ref. 9. The necessary HF solution for the core nucleons and the matrix elements of $\mathcal{U}_{\rm eff}$ with respect to this basis set are taken from Refs. 6 and 9. Both these potentials fail to reproduce the experimental spectra of O^{17}. At this stage it is necessary to mention that we take a single oscillator radial orbit as the HF solution of the core. As can be seen from Refs. 6 and 9, this is not a bad approximation. We use $b=(\hbar/m\omega)^{1/2}=1.76$ F as the oscillator strength parameter in our calculations. Using these core wave func-

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[9] R. Muthukrishnan and M. Baranger, Phys. Letters 18, 160 (1965).

TABLE I. Calculated binding energies of $2s$–$1d$-shell nuclei for the Yale[a] and the nonlocal separable[b] potential are tabulated in the second column. The corresponding experimental values[c] are given in the third column. All the binding energies are relative to the O^{16} binding energy. The calculated binding energies are corrected for the column and the center-of-mass energies.

Nucleus	Calculated binding energies in MeV: Yale potential	Nonlocal separable potential	Experimental binding energies in MeV
^{18}O	6.67	7.96	12.2
^{19}F	15.81	11.37	20.2
^{20}F	18.71	16.22	26.78
^{20}Ne	29.10	19.45	33.27
^{21}Ne	33.48	24.69	40.02
^{22}Na	38.13	28.56	46.77
^{22}Ne	40.79	33.42	50.39
^{23}Na	51.89	38.86	59.18
^{24}Mg	67.99	50.12	70.88

[a] Reference 5.
[b] Reference 9.
[c] L. A. Konig, J. H. E. Mattauch, and A. H. Wapstra, Nucl. Phys. **31**, 18 (1962).

tions and the calculated single-particle energies of O^{17}, the matrix elements of the renormalized interaction in Eq. (11) are calculated for each individual nucleus under investigation. To a first approximation we assume that the outer nucleon orbitals are filled in the order of the harmonic-oscillator orbitals. Thereby the probability of occupation of any shell can be approximated by the ratio of the number of particles in that shell to its total degeneracy. Values thus calculated are used for $A(n,l)$ in Eq. (11). Using the normal procedures, we then carry out the axially deformed HF solution for outer nucleons from Eqs. (9), (10), and (11). The binding energy of a nucleus relative to that of a core nucleus is the projected energy for a total angular momentum $I=K$, obtained from the above HF solution. Since we do not yet know any HF solution for the O^{16} that reproduces its binding energy correctly, it is advisable to present our results relative to that for the O^{16} nucleus. This is necessary in order to find out whether the above approach will reproduce the correct binding energies of the open-shell nuclei if the core HF solution does so for the core nucleus. Thus by presenting the results relative to the O^{16} nucleus we shall be excluding the deviations arising from the core HF solution that we used. Binding energies calculated in this way are presented in Table I. Most of the HF solutions were found to be spherical. One observes from Table I that both potentials fail to provide enough binding, as was the case for O^{16} HF calculations.[6,9] Secondly, the nonlocal separable potential (fitted to reproduce nuclear-matter parameters) gives much less binding than the Yale potential. This shows that even though a potential reproduces the correct nuclear-matter saturation density and the binding, it is not necessary that it should reproduce the binding energies of finite nuclei. One interesting feature of the results presented in Table I is that, all the calculated binding energies (from the Yale potential) differ by about 6 MeV from their respective experimental values.

IV. CONCLUSION

The HF problem for open-shell nuclei is approximated by two separate HF calculations. One is the spherical HF one for the core nucleons, and the other the deformed HF one for the outer nucleons. In this formulation the effect of core polarization naturally comes in through the renormalization of the one-body and two-body potentials of the outer nucleons. This formulation has been applied to calculate the binding energies of $2s$–$1d$-shell nuclei. The calculations are carried out for two sets of potentials, one the Yale potential[5] and the other a nonlocal separable potential.[9] It turns out that the Yale potential gives better binding energies than the nonlocal potential. It is also observed that the calculated Yale potential binding energies differ from their experimental values by an approximately constant value of 6 MeV. We conjecture that the above approach will reproduce the correct binding energies of the open shell nuclei, if the core HF solution used does so for the core nucleus.